

Micellar and Columnar Liquid Quasicrystals

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Our recent high resolution AFM studies of the dodecagonal liquid quasicrystals formed from self-assembled soft micelles will be presented. The results has enabled us to locate the position of each individual micelle, and to examine in more detail of the tiling rules and 3-d arrangement of micelles in such structures. The implications of the findings for current tiling and structural models will be discussed. We present also the discovery of a new kind of liquid quasicrystals which are 2-dimensional and are formed from self-assembled columns. Previous studies on polyphilic T- and X-shaped molecules have revealed their ability to form complex two dimensional honeycomb-like structures of columns with polygonal cross-sections. The polygons found in those structures so far are triangles, squares, rhombi, pentagons, hexagons and, more recently, giant squares and octagons. The quasicrystalline symmetry of the new phase is clearly shown by the "forbidden" 12-fold symmetry of the grazing incidence small-angle X-ray scattering pattern obtained from a thin film. The structure of an approximant at the vicinity of the new LQC columnar phase has been solved, suggesting for the LQC phase a tiling pattern consisting of triangles, squares and pentagons.

*Speaker

Hard-core/square-shoulder quasicrystals

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Reported in various types of micellar suspensions, soft-matter quasicrystals suggest that the mechanisms behind their formation may well rely on rather generic interparticle interactions. We theoretically study a 2D ensemble of particles characterized by a simple pairwise-additive isotropic potential consisting of a hard-core repulsion and a square shoulder, and we show that this two-lengthscale potential does induce a range of bond-ordered phases with non-crystallographic 10-, 12-, 18-, and 24-fold rotational symmetry. The structure of these phases is interpreted in terms of so-called canonical tiles based on core-to-core and shoulder-to-shoulder packed particles, which provide an intuitive geometrical interpretation. We also discuss novel bond-ordered phases with 6-fold symmetry observed in this ensemble.

*Speaker

Gap labeling and energy landscape in a 2D quasicrystal: A microwave experiment

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Two groups in Nice, theoreticians and experimentalists, joined their effort to address the problem of 2D quasicrystals. A microwave realization of a Penrose-tiled lattice using a set of coupled dielectric resonators have been implemented. Using an experimental technique which gives access to both the local density of states and the wavefunctions of the artificial quasicrystal, the gap labeling and the energy landscape of the eigenstates have been measured . At each conducting band is associated wavefunctions with specific symmetry properties. The coupling between resonators being due to a magnetic evanescent field, the lattice is well described by a tight-binding model. Thus, we have been able to develop a perturbative argument to understand the observations.

*Speaker

An ansatz for single electron wavefunctions in quasicrystalline potentials

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A generalization of Sutherland's ansatz wavefunction for the wide variety of continuous and discrete Schrodinger problems in quasicrystals is proposed. Numerical evidence suggests that the ground state of the standard tight-binding models on Ammann and Penrose tilings is described by this ansatz. Relation of these findings to the known results for one-dimensional quasiperiodic potentials is discussed.

*Speaker

Topological properties of Fibonacci quasicrystals : A scattering analysis of Chern numbers

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Topological features of quasicrystals are contained in the spectral labelling of the gaps (the so-called gap labeling theorem) but they have never been directly addressed. In this presentation, Chern numbers will be shown to result from the underlying palindromic symmetry of quasicrystals and a general scattering description is proposed to retrieve them from scattering data. Comparison will be made with other topological systems, e.g. topological insulators.

*Speaker

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Hard sphere packings in cylindrical geometries : curved space analysis

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A general analysis is proposed for dense hard sphere packings inside cylinders. The main observed features, a rich phase structure where chiral and non-chiral configurations alternate when the cylinder radius is varied [1], can be simply described from a template in the positively curved space S^3 , the polytope $\{3,3,5\}$, suitably mapped onto R^3 [2]

We first study the best packing solutions inside toroidal neighbourhoods in S^3 . Using a Hopf fibration analysis, this problem can be greatly simplified into that of a disk covering problem on the sphere S^2 . Upon aligning the fibration with the high order symmetry directions (the polytope has a high order symmetry group with 14400 elements), one already finds typical chiral-non chiral sequences described in the cylinder case

The mapping from these toroidal configurations into periodic cylindrical ones in R^3 is then done by applying a particular (geodesic-like) map, which amounts to "rolling" the polytope onto a tangent R^3 space, along optimal selected geodesic directions of high symmetry. Once the geodesic line is selected, a toroidal neighbourhood is mapped onto R^3 , leading to interesting, slightly deformed, close packed configurations inside a cylinder.

*Speaker

Quasicrystalline Frank-Kasper phases: from metal to micellar structures

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Frank and Kasper phases were introduced more than fifty years ago for metallic alloys [1] for structural description. Surprisingly they allow to describe and predict a huge family of closed packed structures. They optimize the packing of more or less spherical atoms of different sizes such that four atoms always form a tetrahedron not too far from regular one (these phases are also called Tetrahedral Close Packing: TCP).

They can describe metallic alloys but also other materials as for instance clathrates or froth. Recent development in soft matter of the study of the structure of nanoparticles, colloidal spheres or aggregates have show that Frank-Kasper phases occur currently in this domain [2]. There are the possibility of liquid crystals but also of quasicrystalline phases [3].

On important properties of F-K phases is that coordination shells are icosahedra or modification of icosahedra by line defects (disclinations) leading to coordination shells with $Z=12,14,15$ or 16 neighbors. The network of these lines (F-K lines) follows strict conservation rules governing the structure.

The example of quasicrystalline soft phases is interesting from this point of view as it is easy to identify the network of disclination lines: a clear example of a disclination network in a quasicrystalline TCP phase [4].

It is also interesting to see how the dodecagonal symmetry which is observed in the colloidal quasicrystals are related to icosahedral coordination in 3D and to hexagonal packing in 2D.

1. Frank F. C., Kasper J. S., *Acta Crystallogr.* 11 (1958) 184 ; 12 (1959) 483.
2. S. Hajiw, B. Pansu and J-F. Sadoc *ACS Nano* DOI 10.1021/acsnano.5b02216, (2015)
3. Ungar G. and Zeng X., Frank-Kasper quasicrystalline and related phases in liquid crystals. *Soft Matter* 1, (2005) 95–106.
4. R. Mosseri and J-F. Sadoc , *Comptes Rendus Physique* 15, 90-99 (2014).

*Speaker

Diffraction in Aperiodic Order

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The kinematic diffraction of regular model sets and similar highly ordered systems is relatively well understood. In recent years, some progress has been made towards an extension to systems with mixed spectrum. Some of the results are reviewed by means of characteristic examples with singular continuous and absolutely continuous spectral components.

*Speaker

Spectral notions of aperiodic order

Michael Baake * ¹

¹ University of Bielefeld – Germany

The diffraction spectrum of a Delone set in Euclidean space is intimately related to the dynamical or von Neumann spectrum of the corresponding dynamical system under the translation action. Recent developments are reviewed and illustrated for certain examples, including visible lattice points and random inflations.

*Speaker

Beyond Dirac combs

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In any dimension there exist two discrete closed sets S and T which are neither lattices nor quasicrystals and a measure carried by S whose Fourier transform is carried by T . This was discovered by Nir Lev and Alexander Olevskii. The proof of this outstanding result will be sketched. It opens new gates on structured point sets.

*Speaker

Reminiscences of the early days of quasicrystals

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The discovery of quasicrystals has been announced late 1984 through two papers, more than two years after the first observations of five-fold diffraction in rapidly quenched Al₆Mn by D. Shechtman. The two papers differ in several ways. The *Met. Trans* paper[1] showed a numerical model created by Ilan Blech of a very interesting icosahedral glass (a precursor of the random tilings models) that exhibited nicely sharp simulated diffraction patterns. This model was open to criticism and might distract attention from the experiments and was referred to, but left out of the second paper[2] submitted to PRL that was confined to the compelling experimental case alone that challenged several prevailing paradigms of crystallography : the case by itself was strong and sufficient to force a change in thinking the way ordering can occur in solids and how Bragg diffraction was really depending on periodicity.

This talk will give a brief historical perspective of some of the milestones which marked out this long journey from periodic to aperiodic order in crystallography.

1. D. Shechtman and I.A. Blech: *Metall. Trans. A*, 1985, vol. 16A, pp. 1005–12.
2. D. Shechtman, I. Blech, D. Gratias, and J.W. Cahn: *Phys. Rev. Lett.*, 1984, vol. 53, pp. 1951–53.

*Speaker

Brillouin zone labelling for quasicrystals

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We propose a scheme to determine the energy-band dispersion of quasicrystals which does not require any periodic approximation and which directly provides the correct structure of the extended Brillouin zones.

In the gap labelling sight, this allow to transpose the measure of the integrated density-of-states to the measure of the effective Brillouin-zone areas that are uniquely determined by the position of the Bragg peaks. Moreover we show that the Bragg vectors can be determined by the stability analysis of the law of recurrence used to generate the quasicrystal. Our analysis of the gap labelling in the quasi-momentum space opens the way to an experimental proof of the gap labelling itself within the framework of an optics experiment, polaritons, or with ultracold atoms.

*Speaker

Localization of ultracold Bose superfluids in quasiperiodic lattices

Laurent Sanchez-Palencia * ¹

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We report theoretical studies of the physics of Bose superfluids confined in one- and two-dimensional quasiperiodic structures [1,2]. First, we analyze the time-of-flight interference pattern that reveals quasiperiodic long-range order. Second, we study localization effects associated with quasidisorder at the single-body and many-body levels. In one dimension, we demonstrate localization of collective pair excitations both numerically and analytically. For intermediate interaction and quasiperiodic amplitude we find a sharp localization transition, with extended low-energy states and localized high-energy states. Experimental advances are also discussed.

L. Sanchez-Palencia and L. Santos, "Bose-Einstein condensates in optical quasicrystal lattices", Phys. Rev. A 72, 053607 (2005).

S. Lellouch and L. Sanchez-Palencia, "Localization transition in weakly interacting Bose superfluids in one-dimensional quasiperiodic lattices", Phys. Rev. A 90, 061602(R) (2014).

*Speaker

Non-Fermi-Liquid Behavior in Metallic Quasicrystals with Local Magnetic Moments

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⁵ Department of Physics and National High Magnetic Field Laboratory, Florida State University
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Motivated by the intrinsic non-Fermi-liquid behavior observed in the heavy-fermion quasicrystal Au₅₁Al₃₄Yb₁₅, we study the low-temperature behavior of dilute magnetic impurities placed in metallic quasicrystals. We find that a large fraction of the magnetic moments are not quenched down to very low temperatures, leading to a power-law distribution of Kondo temperatures, accompanied by a non-Fermi-liquid behavior, in a remarkable similarity to the Kondo-disorder scenario found in disordered heavy-fermion metals.

*Speaker

Multifractal properties of the Fibonacci chain: Energy Spectrum and Wavefunctions

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We consider the off-diagonal tight-binding model for electrons on the Fibonacci chain, in the limit of strong modulation of the hopping amplitudes. It is well established that this model exhibits multifractal energy spectrum and wavefunctions that imply anomalous diffusion of wavepackets. Using a perturbative real space renormalisation group, we are able to give analytical expressions for the fractal exponents of the energy spectrum and of the wavefunctions which are in extremely good accord with numerical calculations. We also show how the energy and perpendicular position are closely related as far the fractal properties of the wavefunctions are concerned.

*Speaker

Long-range Magnetic Order in Models for Rare Earth Quasicrystals

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We take a two-step theoretical approach to study magnetism of rare earth quasicrystals by considering Ising spins on quasiperiodic tilings, coupled via RKKY interactions. First, we compute RKKY interactions from a tight-binding Hamiltonian defined on the two-dimensional quasiperiodic tilings. We find that the magnetic interactions are frustrated and strongly dependent on the local environment. This results in the formation of clusters with strong bonds at certain patterns of the tilings that repeat quasiperiodically. Second, we examine the statistical mechanics of Ising spins with these RKKY interactions, using extensive Monte Carlo simulations. Although models that have frustrated interactions and lack translational invariance might be expected to display spin glass behaviour, we show that the spin system has a phase transition to low-temperature states with long-range quasiperiodic magnetic order. Additionally, we find that in some of the systems spin clusters can fluctuate much below the ordering temperature.

*Speaker

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Controlled self-assembly of periodic and quasiperiodic cluster crystals.

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We will have heard by now at this conference that quasicrystals form rather robustly in soft-matter systems, consisting of fairly large synthesized molecules, usually exhibiting 12-fold symmetry. If indeed it is possible to design the interaction between particles, it begs to ask whether one can obtain any desired periodic or quasiperiodic structure by self-assembly. I will (partially) answer this question for the interesting example of ultrasoft pair potentials, which are bounded at the origin, and are known to give rise to so-called cluster crystals.

*Speaker

Can soft particles assemble in quasicrystals ?

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Soft particles are excellent candidates for building quasi-crystals since they can adapt their shape and can easily be modeled by local environments. A brief introduction to soft particle systems exhibiting more complex assemblies than FCC or BCC will be presented. Then attention will be focused on gold nanoparticles covered with hydrophobic ligands. Recently(1) the evidence of an unexpected Frank and Kasper phase with hexagonal symmetry has been shown in this system. After describing this phase, its existence will be discussed; it mainly involves the presence of large van der Waals attraction. (1) Evidence for a C14 Frank–Kasper Phase in One-Size Gold Nanoparticle Superlattices Stéphanie Hajiw, Brigitte Pansu, and Jean-François Sadoc

*Speaker

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Colloids in quasiperiodic laser fields: experiments and simulations

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No metallic quasicrystals have been discovered with symmetries other than icosahedral, decagonal and dodecagonal despite many efforts in recent years. Colloids could help to improve insight into this observation since they provide toy systems which can be modified in many different ways: their repulsive interaction can be varied by adding charges and salt; the interference of laser beams may lead to an external optical potential that mimics the influence of a quasiperiodic surface with more symmetries realizable than enumerated above.

Experimental studies have revealed new quasiperiodic stripe phases formed in decagonal and tetradecagonal laser fields as a function of density of the colloids and strength of the field. Unfortunately, experimental studies are restricted in parameter space and do not allow to study arbitrary symmetries due to the large number of laser beam phases that must be controlled. Recently, periodic average structures have also been observed in onedimensional quasiperiodic laser fields.

Quasistatic simulation studies have been able to confirm the experimentally found structures and extend the results to a much larger parameter space and to further symmetries. Thus it was shown that stripe phases occur in all cases and why they are energetically advantageous. Dynamical simulation studies deal with phason flips and diffusion in stripe and quasicrystal phases. Phason flips in the stripe phases could be studied by applying continuous drifts and gradients to the laser field. They stabilize the structures and reduce the number of defects.

With the help of brownian dynamics the behavior of colloids moving in quasiperiodic fields has been analyzed in detail. Flips of particle rows have been observed if the particles are non-interacting. Depending on the direction and velocity of the changing laser field single particles are found moving in phase or in antiphase direction. A classification of the different regimes will be presented. In the case of repellant particles a consecutive decay of the structure is observed for an increasing laser potential shift since the particles can no longer follow the potential minima. This leads to phason drift-induced melting.

*Speaker

Orbital magnetic susceptibility of a quasicrystal

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We describe the motion of electrons on a two-dimensional isometric Rauzy tiling by a tight-binding model. A magnetic field perpendicular to the plane is applied, which couples to the orbital motion of electrons via a Peierls phase in the hopping amplitudes and to the spin via a Zeeman coupling. For several approximants to the quasicrystal, the energy spectrum in a magnetic field is computed numerically with open boundary conditions and has the shape of a Hofstadter butterfly. The grand potential is then obtained at a given temperature and chemical potential and its derivatives allows us to study the orbital magnetic susceptibility as well as the spin susceptibility of the Rauzy tiling. The spin susceptibility is a temperature-smoothed version of the zero-field density of states. The orbital susceptibility has a complicated structure as a function of the chemical potential except near the band edges where it is approximatively described by an effective mass tensor.

*Speaker

AlMnPd and CdYb icosahedral quasicrystal structure families: state of the art and open questions

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For both fundamental intermetallic families of stable quasicrystals, AlMnPd and CdYb, all solved approximant phase structures are tilings of four canonical cells (CCT; Henley 1991), with tiling vertices occupied by distinct clusters, so called "pseudo" Mackay Icosahedron (PMI), and Tsai cluster (TC). Despite some chemical disorder and tricky details due to strong symmetry-breaking of both clusters near their center, the experimentally refined approximant structures can be brought into near-perfect agreement with realistic DFT-level evaluation of total energies, and their energetic stability vs competing crystalline phases can be readily established and understood. For the quasicrystal phase, we have two competing structural scenarios: (1) quasicrystal phase geometry is CCT with space tiled by four canonical cells, ABCD. The tiling is random ensemble or a particular quasiperiodic tiling; (2) the largest canonical cell "D" is unstable, and besides ABC tiles the quasicrystal structure includes some other cells, or specific "superclusters" or even alternative fundamental clusters. I will discuss likelihood of the two scenarios for prominent quasicrystal forming systems.

*Speaker

Structure and dynamics of quasicrystals.

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The relation between the quasicrystal atomic structure and its physical properties is a long standing and still open question. The presentation will illustrate our current understanding of the dynamics of quasicrystals, and in particular phason modes, an excitation that is specific to all aperiodic crystals (1). Experiments for icosahedral quasicrystals in the Tsai type CdYb system will be presented and compared to the periodic approximant. The essential role of clusters and icosahedral symmetry breaking will be outlined.

Open questions in this field will be addressed at the end of the presentation.

1 T. Janssen, G. Chapuis, and M. de Boissieu, *Aperiodic Crystals. From modulated phases to quasicrystals* (Oxford University Press, Oxford, 2007).

*Speaker